Effect of X-Ray Diffractometer Geometrical Factors on the Centroid Shift of a Diffractic Line for Stress Measurement

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Expressions for the centroid shift of a diffraction lino duo to geometrical factors have been deduced for a diffractometer case in which the specimen surface is inclined to the x-ray beam at an arbitrary angle. Such a geometry is encountered in the determination of residual stress using a diffractometer. The effects of the centroid shift of a diffraction line due to geometrical factors on the stress derived from the diffractometer measurements have teen discussed.

I. INTRODUCTION

In order to achieve high resolution and high count rate simultaneously, the modern diffractometers employ Bragg-Brentano focusing using a line source and a pair of Soller slits. The focusing conditions in practice deviate from the ideal in the following respects[1]: (a) The specimen surface does not possess the curvature required for focusing. (b) The x rays penetrate into the specimen and diffracted beam of appreciable intensity occurs from the part of the specimen which does not lie on the diffractometer axis. (c) The source and the receiving slit have finite widths. (d) The incident beam has appreciable axial divergence. Further deviations from the ideal conditions may be caused by poor adjustment of the diffractometer with respect to the x-ray source and oi the specimen with respect to the diffractometer axis.

Any departure from the ideal conditions of focusing tends to distort the diffraction line profile. A measure of the position of a diffraction line is either the peak maximum or the centroid. In practice, determining the peak position of a line is easier than the centroid. However, mathematically, the effect of geometrical aberrations on the centroid can be more easily calculated since a diffraction maximum is the convolution[2-5] of the profiles due to individual sources of aberrations; and in such a case the centroid is the sum of the centroids of the individual profiles.

The effect of these aberrations on a diffraction maximum has been considered[4-13] in detail for the normal diffractometer condition.

However, for the determination of residual[14] macrostresses in polycrystalline solids using an x-ray diffractometer, it is essential to set the specimen making an arbitrary angle to the x-ray beam. In such a case, the diffracted beam is focused (Fig. 1) at a point whose distance from the diffractometer axis is given by

$$R = S \sin(\theta - \psi)/\sin(\theta + \psi), \quad (1)$$

where S is the distance of the source from the diffractometer axis, B is the Bragg angle, and ψ is the angle between the specimen-surface normal and the reflecting-plane normal. In this paper, we have extended Wilson's[13] method to derive expressions for the centroid shift of diffraction line due to geom rical factors for a geometry shown in Fig. 1. T errors introduced by the centroid shift in the ex perimental values of stresses have also been di cussed.

II. BASIC EQUATIONS

In this section, the basic approach of Wilson's method[13] as modified for the present case has b summarized.

A. Choke of Axes

A plane normal to the diffractometer axis and p ing through the center of gravity of the source a viewed from the axis defines the equatorial plan The divergence of the incident x-ray beam in th piano is termed equatorial divergence. The div gence in a piano containing the diffractometer a; and the center of the line source is termed axi divergence. The point of intersection of the axi the equatorial piano is taken as the origin of coo dinates (0 in Fig. 2). The vector $\vec{S}$ (joining A tc in the equatorial plane defines an ideal incident The ideal diffracted ray is defined by a vector $\vec{R}$ The length of the vector is fixed by Eq. (1). Th rection of $\vec{R}$ is defined by the projection on the torial plane of the line joining O to B', the cent gravity of the receiving slit. In a properly adju Instrument, B' will coincide with B.

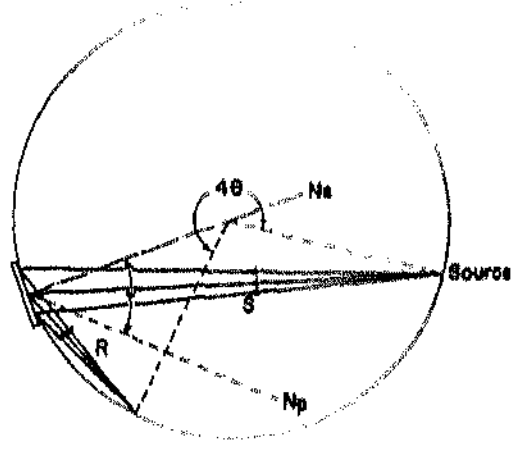

FIG. 1. Focusing geometry when the x-ray beam 1 inclined to the specimen at an arbitrary angle.

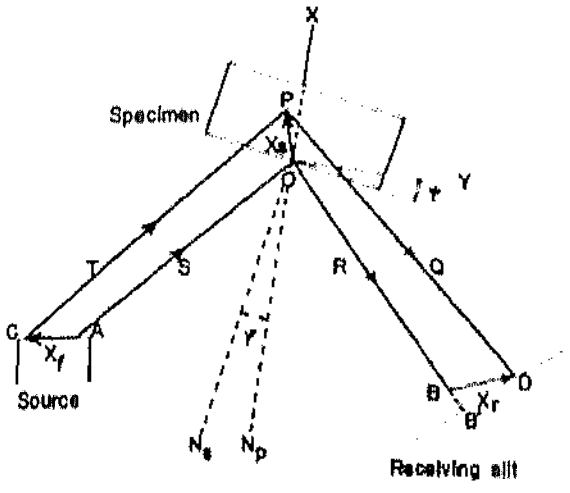

FIG. 2. Definition of the various vectors.

The X and Y axes are chosen in the equatorial plane such that they bisect the angle between $\vec{S}$ and $\vec{H}$. Z axis is taken perpendicular to X and V,

A crystallite at O will diffract a ray from ,4, in the direction *on* when the diffractometer is set at 2θ, i.e., the angle between $\vec{H}$ and $\vec{R}$ is 2". Another crystallite flituatt*cl at a point P in thf* specimen will diffract a ray T, from C along PD ($\vec{Q}$) when the diffractometer setting is $2\theta'$. $2\theta'$ differs from 2θ by tt small quantity 2ϵ such that $2\theta' = 2\theta - 2\epsilon$.

D. Expression for 2ϵ

Let us consider three vectors, $\vec{x}_s$, $\vec{x}_f$, and $\vec{x}_r$, which define a point in the specimen, the source and the receiving slit, respectively. We shall now derive an expression for 2ϵ in terms ttf these vectors. From Fig. 2 H is clear that

$$\vec{T} = \vec{S} + \vec{x}_s - \vec{x}_f \tag{2}$$

and

$$\vec{Q} = \vec{R} + \vec{x}_r - \vec{x}_s . \tag{3}$$

Since $|(\vec{x}_s - \vec{x}_f)|/S$ and $|(\vec{x}_r - \vec{x}_s)|/R$ are small as compared to unity, neglecting the terms in small quantities having powers more than 2, we get

$$T^{-1} = S^{-1}\{1 - S^{-2}\vec{S}\cdot(\vec{x}_s - \vec{x}_f) + S^{-2}|(\vec{x}_s - \vec{x}_f)|^2 + \tfrac{1}{2}S^{-2}|\vec{S}\cdot(\vec{x}_s - \vec{x}_f)|^2\} \tag{4}$$

and

$$Q^{-1} = R^{-1}\{1 - R^{-2}\vec{R}\cdot(\vec{x}_r - \vec{x}_s) - \tfrac{1}{2}R^{-2}|(\vec{x}_r - \vec{x}_s)|^2 + \tfrac{1}{2}R^{-2}|\vec{R}\cdot(\vec{x}_r - \vec{x}_s)|^2\}. \tag{5}$$

Since the angle between T and $\vec{Q}$ is 2θ, we have

$$\cos 2\theta = T^{-1}Q^{-1}\vec{T}\cdot\vec{Q}. \tag{6}$$

We choose orthogonal components of vectors $\vec{x}_s$, $\vec{x}_f$, and $\vec{x}_r$ ftg follows. The components x_s and y_s of $\vec{x}_s$ are in the equatorial plane and, respectively, perpendicular and parallel to the specimen surface. x_f and y_f are the components of $\vec{x}_f$ in the equatorial plane and, respectively, parallel and perpendicular to $\vec{S}$. x_r and y_r are in the equatorial plane and, respectively, parallel and perpendicular to $\vec{R}$. All the z components are along Z axis.

At this stage, it is necessary to consider the relative magnitudes of the various vector components so that a meaningful approximation may be made. In practice, we have the following conditions governing the relative magnitudes of the components of the vectors x_s, x_f, and $\vec{x}_r$:

(a) Since the x-ray beam is strongly absorbed in the specimen, the points with large x_s do not contribute appreciably to the diffracted intensity and thus only the points with $x_s \sim y_s$ and z_s need be considered.

(b) Normally, a line source is used with powder diffractometer. The use of the Soller slit limits the effective value of z_f and is of the order of the separation between the parallel foils of the Soller slit (about 0.5 mm). The focal spot is normally 1 x 10 mm and when it is viewed at a takeoff angle about 3°–5°, $x_f \simeq 1$ mm and $y_f \simeq 0.05$ mm. Thus, in general, $y_f \sim x_f \sim z_f$.

(c) Similar ttrpmentd show that $y_r \sim z_r$ and x_r is nearly a constant.

On substituting in Eq. (6) the values for $\vec{T}$, $\vec{Q}$, T^{-1}, and Q^{-1} from Eqs. (2)–(5) and retaining only the significant terms wo get the following expression for 2ϵ:

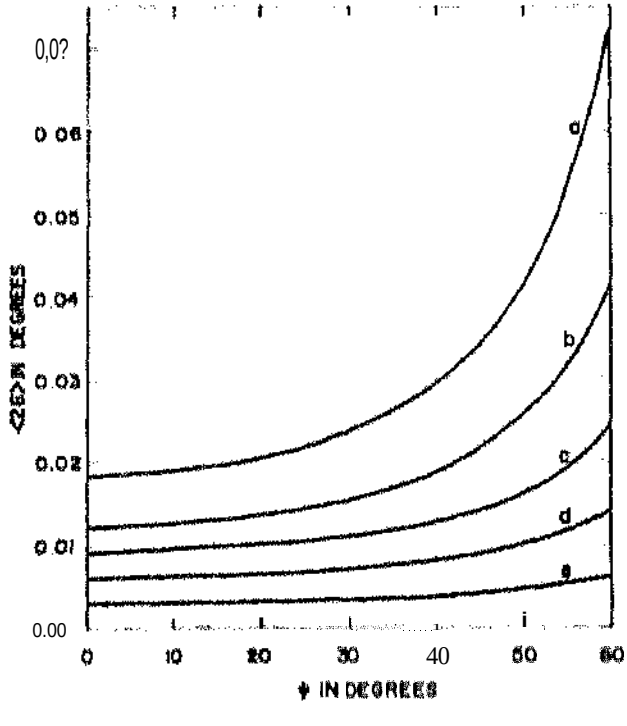

FIG. a. Plot of $(2\epsilon)_s + (2\epsilon)_g$ vs ϕ. μ–WO cm^{-1} and $S = 17$ em have been used to calculate $(2\epsilon)_g$. (a) $\theta = 75°$, $2\alpha = 4°$, (b) $\theta = 80°$, $2\alpha = 4°$, (c) $\theta = 75°$, $2\alpha = 2°$, (d) $\theta = 80°$, $2\alpha = 2°$, (e) $\theta = 85°$, $2\alpha = 2°$. The curve for $\theta = 85°$ and $2\alpha = 4°$ almost overlaps with (d).

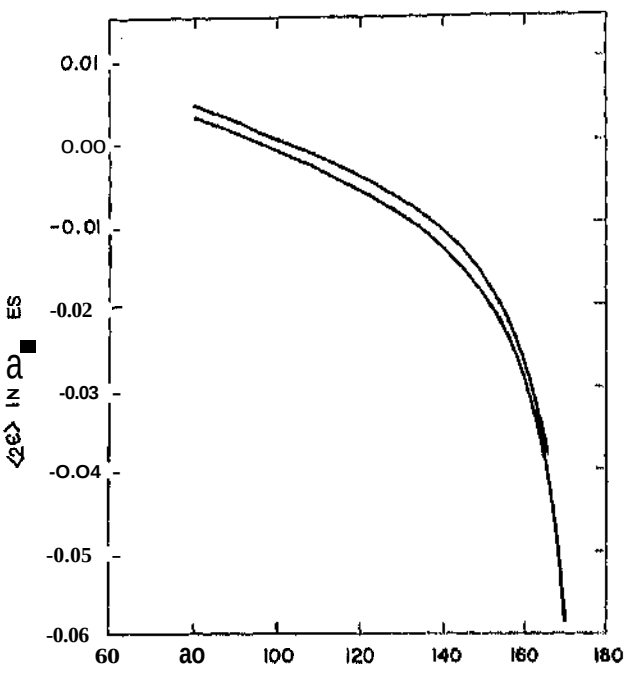

FIG. 4. Plot of $\langle 2\epsilon\rangle_{\text{axial}}$ vs 2θ for $q = 1.4$. Upper curve $\psi = 0°$. Lower curve $\psi = 30°$.

$$2\epsilon = \eta^{-1}S^{-1}\{x_s[\cos(\varphi - \psi) + \eta\cos(\varphi + \psi)] + y_r + \eta y_f\}$$
$$+ S^{-2}[y_s^2\eta^{-1}\sin 2\varphi - x_f y_s \sin(\varphi + \psi) - \eta^{-2}x_r y_s \sin(\varphi - \psi)]$$
$$+ \eta^{-1}S^{-2}\{z_s^2[1 + \tfrac{1}{2}(\eta + \eta^{-1})\cos 2\varphi]\csc 2\varphi + \tfrac{1}{2}z_r^2\eta^{-1}\cot 2\varphi$$
$$+ \tfrac{1}{2}z_f^2\eta\cot 2\varphi - z_r z_s(1 + \eta^{-1}\cos 2\varphi)\csc 2\varphi$$
$$+ z_r z_f \csc 2\varphi - z_f z_s(1 + \eta\cos 2\varphi)\csc 2\varphi\}, \quad (7)$$

where

$$\eta = \sin(\theta - \psi)/\sin(\theta + \psi).$$

III. CENTROID SHIFT

A. Equatorial Terms

We shall first consider the terms containing equatorial components.

The terms $y_r/\eta S$ and V^s represent the displacements due to finite width of the source and the receiving slit. The axes of coordinates have been so chosen that

$$\langle y_f\rangle = \langle y_r\rangle = 0.$$

These terms therefore do not lead to any displacement of the centroid.

The term in x_s leads to displacement due to various factors. These include (a) the displacement of the specimen surface from the axis of the diffractometer, (b) tilt of the specimen surface with the diffractometer axis, (c) missetting of I of the 2 : 1 ratio and the variation of 2: 1 r angle, and (d) the finite absorption of the x beam in the specimen.

The displacement of the specimen surface diffractometer axis displaces centroid of a tion line from its true position. The centre of a diffraction lino due to a displacement l specimen surface from the axis is given by

$$\langle 2\epsilon\rangle_1 = l\sin 2\theta/S\sin(\theta - \psi). \quad (8)$$

t is taken to be positive if the diffractomete lies outside the specimen and negative othe

The tilt of the specimen with respect to diffi oter axis does not lead to any displacement small broadening. Similarly, the missetting zero of 2: 1 ratio leads only to broadening.

Duo to the finite absorption of x rays in the men, diffractedbeam of appreciable intenst arise from the material beneath the surface specimen or, in other words, from the regi is displaced from the axis of the diffractome displacement of the centroid caused by this J tained by taking the weighted average of the in x_s in 15q, (7) and is given by

$$\langle 2\epsilon\rangle_2 = \eta^{-1}S^{-1}[\cos(\varphi - \psi) + \eta\cos(\varphi + \psi)]\langle x_s\rangle, \quad (9)$$

where

$$\langle x_s\rangle = \int_0^t x_s e^{-\mu m x_s} dx_s / \int_0^t e^{-\mu m x_s} dx_s,$$

where μ is the linear absorption coefficient t specimen for the radiation used, $m = \csc(\varphi - \psi) + \csc(\varphi + \psi)$, and t is the specimen thickness.

On evaluating the integrals, we get

$$\langle x_s\rangle = [1 - \mu m t(e^{\mu m t} - 1)^{-1}]/\mu m. \quad (10)$$

Even if μ is moderately large, the x-ray bea absorbed in the specimen within fractions of and therefore the thickness of the specimen e countered in practice can be taken as infinite. tends toward infinity, tho second term betwee square brackets tends toward zero. Thus, fo specimen of infinite thickness, we have

$$\langle x_s\rangle = 1/\mu m. \quad (11)$$

On substituting the value of $\langle x_s\rangle$ from Eq. (11) (0), we get

$$\langle 2\epsilon\rangle_2 = (\eta\mu m S)^{-1}[\cos(\varphi - \psi) + \eta\cos(\varphi + \psi)]. \quad (12)$$

In case μ is small, *Eq.* (10) instead of (11.) m used for tho value of $\langle x_s\rangle$. Additional complica which arise if the absorption coefficientis ver have been considered by Milberg.[16] We shall n consider this case as it la not commonly encou tered in practice.

The shift of eentroid due to term in y_s^2 is given

$$\langle 2\epsilon\rangle_3 = \eta^{-1}S^{-2}\sin 2\varphi\langle y_s^2\rangle. \quad (13)$$

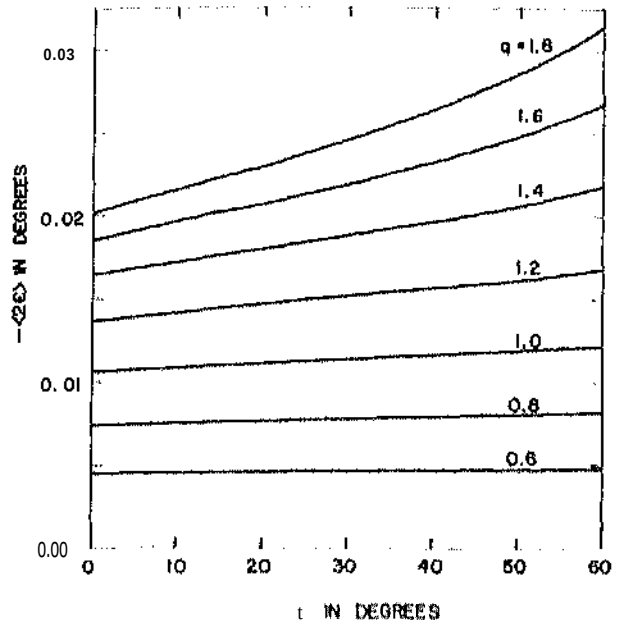

FIG. ti. Mot of $\langle 2\epsilon \rangle_{axial}$ vu ϕ for $\theta = 75°$, $2P = 1$ cm and $S = 17$ cm.

If wo assume a uniform distribution of intensity in the primary beam, then

$$\langle y_s^2 \rangle = \int_{-A_2}^{A_2} y_s^2 dy_s / \int_{-A_1}^{A_1} dy_s,$$
$$\langle y_s^2 \rangle = \tfrac{1}{3}(A_2^2 - A_1 A_2 + A_1^2). \tag{14}$$

Since the equatorial divergence 2α IH small, wo have

$$A_1 \simeq A_2 \simeq S\alpha/\sin(\varphi + \psi).$$

On substituting the values of A_1 and A_2, wo get

$$\langle 2\epsilon \rangle_3 = \frac{1}{3} \frac{\alpha^2 \sin 2\varphi}{\sin(\varphi + \psi)\sin(\varphi - \psi)}. \tag{15}$$

Tho term in $x_f y_s$ does not contribute to the rilKplu.eo» ment of centroid since the axis has been HO chosen that $\langle x_f \rangle = 0$ and there is no correlation between x_f and y_s.

Tho term in $x_r y_s$ will contribute to the displacement of centroid and the broadening. These contributions arise due to the ftu-t that the center of gravity of the illuminated area does not lie on the diffractometer axis and there is small error in the adjustment of the position of the receiving slit on the detector arm, By careful adjustment, these errors can be reduced to about 0. 1 tun. With these values, the displace- ment of the centroid should be less than

$$\langle 2\epsilon \rangle_4 = 0.01(\eta S)^{-2} \sin(\varphi - \psi). \tag{10}$$

B. Axial Terms

We shall now derive an expression for the centroid shift arising from the axial terms. The axial terms in Eq, (?) can bo rewritten

$$\langle 2\epsilon \rangle_{axial} = \tfrac{1}{2}\delta^2 \cot 2\varphi + \tfrac{1}{2}\nu^2 \cot 2\varphi - \delta\nu \csc 2\varphi, \tag{17}$$

where

$$\delta = (z_d - z_f)/S \tag{1}$$

and

$$\nu = (z_r - z_s)/\eta S. \tag{1}$$

6 and ν represent the angles which incident and the diffracted rays make with the equatorial plane. We shall consider the case of two Soller slits, one in th the incident beam and the other in the diffracted beam. The Sollet slits limit the maximum axial divergence to A and reduce the intensity by a factor $(1 - |\delta|/\Delta)$ of the rays which make an angle 6 with the equatorial plane; A is equal to the separation between the foils of the Sailer slits divided by the length of the foil.

The displacement of the centroid is given by

$$\langle 2\epsilon \rangle_{axial} = N/D, \tag{20}$$

whore

$$N = \int\int\int \langle 2\epsilon \rangle_{axial}(1 - |\delta|/\Delta)(1 - |\nu|/\Delta)\, d\nu\, d\delta\, d\varphi \tag{21}$$

and

$$D = \int\int\int (1 - |\delta|/\Delta)(1 - |\nu|/\Delta)\, d\nu\, d\delta\, d\varphi. \tag{22;}$$

It IH sufficient[10] to consider only the positive value of 0 with both positive and negative values for ν. $f>$ is identical with z_s. Following Pike,[10] wo introduce a parameter q which is defined as

$$\Delta S = qP,$$

whore $2P$ is the axial dimension of the specimen. We shall confine our attention only to the case in which the axial dimensions of the focus, specimen, and the receiving slit are all equal. In practice, one can turn the specimen such that the surface normal

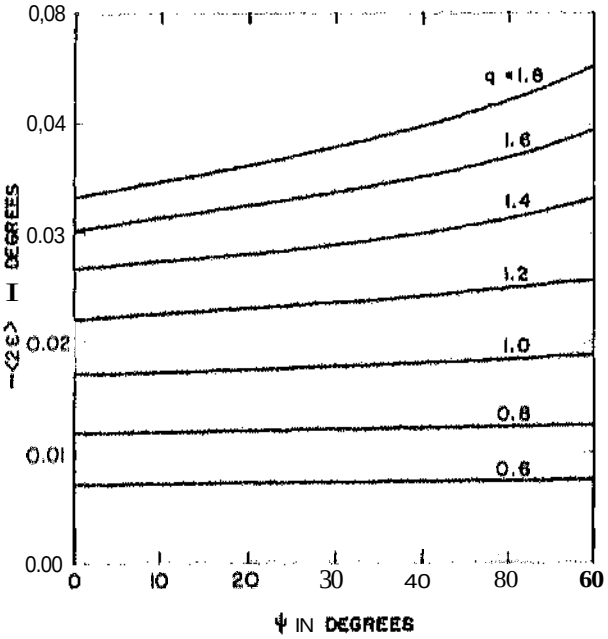

FIG. 6. Wot of $\langle 2\epsilon \rangle_{axial}$ vs ψ ftw $\theta = 80°$, $2P = 1$ cm and $S = 17$ cm.

TABLE I. Estimation of $\Delta\sigma$ [a] for a few materials, $S = 17$ cm, $q = 1.4$, and $2P = 1$ cm have been used in the calculations. These values are for a Norelco powder diffractometer.

Material	Radiation (hkl)	$2\theta°$	$2\alpha°$	$K_{(0-45)}$ ksi/°$\Delta 2\theta$	$\langle 2\epsilon\rangle_0 - \langle 2\epsilon\rangle_{45}$	$\Delta\sigma$	$K_{(0-60)}$ ksi/°$\Delta 2\theta$	$\langle 2\epsilon\rangle_0 - \langle 2\epsilon\rangle_{60}$	$\Delta\sigma$
Steel AISI 4340	Cr$K\alpha$ (211)	156	4	120	−0.0073	−0.8760	HO	−0.0305	−3.4400
			1		+0.0029	+0.3480		+0.0032	+0.2560
Titanium alloy Ti-6Al-4V	Cu$K\alpha$ (2133)	150	}	70	-0.0111	−0.7770	47	−0.0462	−2.1714
					+0.0024	+0.1680		+0.0017	+0.0799
Aluminum alloy 7079-T611	Cr$K\alpha$ (311)	140	4	"	−0.0198	−0.9900	33	−0.0924	−3.0492
			1		+0.0010	+0.0500		−0.0029	−0.0957
Aluminum alloy 7079-T611	Cu$K\alpha$ (333)	162	I	–	−0.0045	−0.0900	13	−0.0104	−0.2522
					+0.0028	+0.0560		+0.0036	+0.0468

[a] In calculating $\langle 2\epsilon\rangle_0$ and $\langle 2\epsilon\rangle_\psi$, same value of 2θ has been used. The numerical values therefore, correspond to a limiting case when the specimen is stress free. In the presence of any stress, 2θ and $2\theta_\psi$ will differ slightly.

moves either towards the source (as shown in Fig. 1) or away from it; the position of the receiving slit moves respectively closer to or farther from the diffractometer axis. For various practical reasons, the former setting is chosen. This gives $\eta \leq 1$. We shall, therefore, consider only $\eta \leq 1$ in the further discussions. The expressions for $\langle 2\epsilon\rangle_{axial}$ for the various cases are given in the Appendix.

IV. DISCUSSION

The total displacement of the centroid of a diffraction line is given by the sum of the displacements due to the various terms in Eq. (7). Among the contributions arising from the equatorial terms, $\langle 2\epsilon\rangle_1$ and $\langle 2\epsilon\rangle_4$ can be made negligible by the proper adjustment of the specimen and diffractometer. The main sources of displacement of the centroid are then, the specimen transparency and the divergence of the beam. A plot of $\langle 2\epsilon\rangle_2 + \langle 2\epsilon\rangle_3$ against * is shown in Fig. 3 for a few fl and 2θ values. μ 140 cm^{-1} and $S = 17$ cm have been used in the computation of $\langle 2\epsilon\rangle_2$. Both $\langle 2\epsilon\rangle_2$ and $\langle 2\epsilon\rangle_3$ are positive and therefore the total displacement is towurtUt low θ value. Since μ occurs in the denominator [Eq. (12)], $\langle 2\epsilon\rangle_2$ be-

TABLE II. Limits of δ, ν, and p used in Eqs. (21) and (22).

	(I) $q \geq 2$ and $\eta q \geq 2$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq +P$	$-(P+p)/\eta S \leq \nu \leq (P-p)/\eta S$
	(II) $q \geq 2$ and $1 \leq \eta q \leq 2$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq A$
$0 \leq \delta \leq (P+p)/S$	$P(1-\eta q) \leq p \leq -P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq (P-p)/\eta S$
$0 \leq \delta \leq (P+p)/S$	$-P(1-\eta q) \leq p \leq +P$	$-\Delta \leq \nu \leq (P-p)/\eta S$
	(III) $q \geq 2$ and $\eta q \leq 1$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq -P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq A$
$0 \leq \delta \leq (P+p)/S$	$-P(1-\eta q) \leq p \leq P(1-\eta q)$	$-A \leq \nu \leq A$
$0 \leq \delta \leq (P+p)/S$	$P(1-\eta q) \leq p \leq +P$	$-A \leq \nu \leq (P-p)/\eta S$
	(IV) $1 \leq q \leq 2$ and $1 \leq \eta q \leq 2$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq A$
$0 \leq \delta \leq (P+p)/S$	$P(1-\eta q) \leq p \leq -P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq (P-p)/\eta S$
$0 \leq \delta \leq (P+p)/S$	$-P(1-\eta q) \leq p \leq -P(1-q)$	$-\Delta \leq \nu \leq (P-p)/\eta S$
$0 \leq \delta \leq \Delta$	$-P(1-q) \leq p \leq +P$	$-\Delta \leq \nu \leq (P-p)/\eta S$
	(V) $1 \leq q \leq 2$, $\eta q \leq 1$ and $(q+\eta q) \geq 2$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq -P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq \Delta$
$0 \leq \delta \leq (P+p)/S$	$-P(1-\eta q) \leq p \leq P(1-\eta q)$	$-\Delta \leq \nu \leq \Delta$
$0 \leq \delta \leq (P+p)/S$	$P(1-\eta q) \leq p \leq -P(1-q)$	$-\Delta \leq \nu \leq (P-p)/\eta S$
$0 \leq \delta \leq \Delta$	$-P(1-q) \leq p \leq P$	$-\Delta \leq \nu \leq (P-p)/\eta S$
	(VI) $1 \leq q \leq 2$ and $\eta q \leq 1$ and $(q+\eta q) \geq 2$	
$0 \leq \delta \leq (P+p)/S$	$-P \leq p \leq -P(1-\eta q)$	$-(P+p)/\eta S \leq \nu \leq \Delta$
$0 \leq \delta \leq (P+p)/S$	$-P(1-\eta q) \leq p \leq -P(1-q)$	$-\Delta \leq \nu \leq \Delta$
$0 \leq \delta \leq \Delta$	$-P(1-q) \leq p \leq P(1-\eta q)$	$-\Delta \leq \nu \leq \Delta$
$0 \leq \delta \leq \Delta$	$P(1-\eta q) \leq p \leq P$	$-\Delta \leq \nu \leq (P-p)/\eta S$
	(VII) $q \leq 1$ and $\eta q \leq 1$	
	Same as (VI)	

comes appreciable only when ψ is low. For a given value of θ and 2α, the displacement of the centroid is minimum at $\psi = 0$ and increases with the increasing value of ψ.

The expressions (given in the Appendix) for the centroid shift due to axial divergence are more complicated. The nature of $\langle 2\epsilon \rangle_{axial}$ is best understood with the help of Figs. 4 fl. Figure 4 shows the variation of $\langle 2\epsilon \rangle_{axial}$ with 2θ for $\eta = 1.4$ and $\psi = 0°$ and $\psi = 30°$. It is seen that for low 2θ values, $\langle 2\epsilon \rangle_{axial}$ is positive and decreases with the increasing value of 2θ, passes through zero, and becomes negative for high 2θ values. Thus, for high-angle reflections which are mostly used in stress measurement work, the shift is towards high 2θ value. Figures fi and fl show the variation of $\langle 2\epsilon \rangle_{axial}$ with ψ for $\theta = 75°$ und 80°, respectively.

V. EFFECT ON STRESS MEASURIM! NI

It is interesting to estimate the errors introduced by the centroid Hhlft of a diffraction line, in the measured values of stresses. First, we shall consider the effect on the stress factor, which is determined by measuring $(2\theta_0 - 2\theta_\psi)$ as a function of stress σ, applied to a test specimen.[14] Within the elastic limits a plot of $(2\theta_0 - 2\theta_\psi)$ vs σ is a straight line. The slope $d\sigma/d(2\theta_0 - 2\theta_\psi)$ of the line gives the stress factor K. The displacement of the diffraction line will introduce an error $\Delta\langle 2\epsilon \rangle_0 - \langle 2\epsilon \rangle_\psi$ in $(2\theta_0 - 2\theta_\psi)$. The error, therefore, will shift the line in σ vs $(2\theta_0 - 2\theta_\psi)$ plot, parallel to $(2\theta_0 - 2\theta_\psi)$ axis. This will appear as a spurious residual stress of magnitude $K(\langle 2\epsilon \rangle_0 - \langle 2\epsilon \rangle_\psi)$. The conclusions are based on the approximation which does not introduce appreciable errors, that $\langle 2\epsilon \rangle_0 - \langle 2\epsilon \rangle_\psi$ is constant at different stress levels. Thus, to a good approximation the determination of K is not affected by the centroid shift.

The effect of the centroid shift on the determination of stress is such that

$$\sigma_{true} = K(2\theta_0 - 2\theta_\psi) + K(\langle 2\epsilon \rangle_0 - \langle 2\epsilon \rangle_\psi),$$

$$\sigma_{true} = \sigma_{obs} + \Delta\sigma.$$

For a few materials, $\Delta\sigma$ has been estimated and results are summarized in Table 1. It is seen that $\Delta\sigma$ is small if the measurement at $\psi = 0°$ and $\psi = 45°$ are made and 2α is 1°.

The corrections become appreciable for $2\alpha = 4°$. The measurements are often made at $\psi = 0°$ and $\psi = 60°$ to achieve better sensitivity. The corrections in this case become appreciable especially for $2\alpha = 4°$.

CONCLUSION

The expressions derived in this paper enable us to calculate the shift of the centroid of a diffraction maximum for a diffractometer tfemnetry used in the determination of residual stresses. This analysis may serve as a useful guideline in selecting various parameters such as the equatorial and the axial divergences to minize the errors. In cases this cannot be done because either it results in a considerable drop of intensity or the proper sizes of slit systems are not readily available, tiw errors can be calculated and a correction applied if found appreciable.

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APPENDIX

The limits of the integrals in Eqs. (21) and (22) under various conditions are given in Table II. On evaluating the integrals we find that the expressions for $\langle 2\epsilon \rangle_{axial}$ are identical for cases II and III and for IV and V. Thu expressions (with u notation $\eta q = u$) for thu various cases are given below:

Case I, $q > 2$ and $\eta > 2/q$:

$$\langle 2\epsilon \rangle_{axial} = (I^0/N^0)\{[\eta^{-1}(-\tfrac{1}{12}u + \tfrac{1}{8}u^2) + \eta^{-2}(\tfrac{3}{160} - \tfrac{1}{48}u) + \eta^{-3}(-\tfrac{1}{48}u + \tfrac{1}{8}u^2) + (\tfrac{3}{160} - \tfrac{3}{8}u)]\cot 2\psi - [\eta^{-1}(\tfrac{1}{8}u - \tfrac{1}{8}u^2) + \eta^{-2}(-\tfrac{1}{160} + \tfrac{1}{8}u)]\csc 2\psi\}\{\eta^{-1}(-\tfrac{1}{8}u + u^2) + \tfrac{1}{16} - \tfrac{1}{8}u)\}^{-1}. \quad (23)$$

Case II, $q > 2$ and $\eta < (2/q - 1)$:

$$\langle 2\epsilon \rangle_{axial} = (I^0/N^0)\{[\eta^{-1}(\tfrac{1}{48}u^2 - \tfrac{1}{384}u^4) + \eta^{-2}(-\tfrac{1}{8}u^2 + \tfrac{1}{48}u^3 - \tfrac{1}{48}u^4 + \tfrac{1}{384}u^5) + \eta^{-3}(\tfrac{3}{8}u - \tfrac{3}{16}u^2 + \tfrac{1}{16}u^3 - \tfrac{1}{48}u^4) + (-\tfrac{3}{8} + \tfrac{3}{8}u - \tfrac{1}{8}u^2 + \tfrac{1}{48}u^3 - \tfrac{1}{384}u^4 + \tfrac{1}{3840}u^5)]\cot 2\psi - [\eta^{-2}(-\tfrac{1}{48}u^2 + \tfrac{1}{48}u^3 - \tfrac{1}{96}u^4) + \eta^{-3}(\tfrac{1}{8}u^2 - \tfrac{1}{16}u^3 + \tfrac{1}{48}u^4 - \tfrac{1}{384}u^5)]\csc 2\psi\}/[\eta^{-1}(2u - \tfrac{1}{8}u^2) + (-\tfrac{1}{8} + \tfrac{1}{8}u - \tfrac{1}{48}u^2 + \tfrac{1}{48}u^3)]. \quad (24)$$

Case III, $1 < q < 2$ and $\eta > (2/q - 1)$:

$$\langle 2\epsilon \rangle_{axial} = (I^0/N^0)\{[\eta^{-2}\tfrac{1}{384}u^3 + \eta^{-3}(-\tfrac{1}{384}u^4 + \tfrac{1}{384}u^5) + \eta^{-4}(\tfrac{3}{384}u^4 - \tfrac{1}{384}u^5 + \tfrac{1}{384}u^6) + \eta^{-5}(-\tfrac{1}{8}u^3 + \tfrac{1}{16}u^4 - \tfrac{1}{48}u^5 + \tfrac{1}{384}u^6) + \eta^{-6}(\tfrac{1}{8}u - \tfrac{1}{8}u^2 + \tfrac{1}{16}u^3 - \tfrac{1}{48}u^4 - \tfrac{1}{384}u^5) + \eta^{-4}(-\tfrac{3}{8} + \tfrac{1}{4}u - \tfrac{1}{16}u^2 + \tfrac{1}{16}u^3 + \tfrac{1}{128}u^4) + \eta^{-5}u^{-1}(\tfrac{1}{16} - \tfrac{1}{16}u + \tfrac{1}{16}u^2 - \tfrac{1}{48}u^3) + \eta^{-6}u^{-1}(-\tfrac{1}{384} + \tfrac{1}{128}u - \tfrac{1}{128}u^2 + \tfrac{1}{128}u^3 - \tfrac{1}{384}u^4 + \tfrac{1}{3840}u^5) + \eta^{-4}u^{-1}(\tfrac{1}{16} - \tfrac{1}{16}u + \tfrac{1}{16}u^2 - \tfrac{1}{48}u^3) + u^{-2}(-\tfrac{1}{384} + \tfrac{1}{128}u - \tfrac{1}{96}u^2 + \tfrac{1}{128}u^3 - \tfrac{1}{384}u^4 + \tfrac{1}{3840}u^5)]\cot 2\psi - [\eta^{-3}\tfrac{1}{384}u^3 + \eta^{-4}(\tfrac{1}{384}u^4 - \tfrac{1}{384}u^5)$$

$$+\eta^{-6}(-\tfrac{1}{10}a^3+\tfrac{1}{20}a^4)+\eta^{-5}(\tfrac{2}{5}a^2-\tfrac{1}{6}a^3+\tfrac{1}{72}a^5)+\eta^{-4}(-\tfrac{2}{9}a+\tfrac{2}{9}a^2-\tfrac{1}{10}a^4)+\eta^{-3}a^{-1}(\tfrac{8}{45}-\tfrac{4}{15}a+\tfrac{2}{5}a^3-\tfrac{1}{6}a^4+\tfrac{1}{30}a^5)$$
$$+\eta^{-1}a^{-2}(-\tfrac{32}{315}+\tfrac{8}{45}a-\tfrac{2}{9}a^3+\tfrac{2}{9}a^4-\tfrac{1}{10}a^5+\tfrac{1}{45}a^6-\tfrac{1}{252}a^7)\}\csc 2\varphi\}/[\eta^{-5}\tfrac{1}{20}a^3+\eta^{-4}(-\tfrac{1}{12}a^2+\tfrac{1}{24}a^3)$$
$$+\eta^{-3}(\tfrac{1}{3}a-\tfrac{1}{3}a^2-\tfrac{1}{12}a^3)+\eta^{-2}(-\tfrac{2}{3}+a+\tfrac{1}{2}a^2)+\eta^{-1}a^{-1}(\tfrac{2}{3}-\tfrac{4}{3}a+a^2-\tfrac{1}{3}a^3)+\text{rt}^{-8}(-\tfrac{1}{15}+\tfrac{2}{5}a-\tfrac{2}{5}a^2+\tfrac{1}{3}a^3-\tfrac{1}{12}a^4$$
$$+\tfrac{1}{60}a^5)]. \tag{25}$$

ase IV. $q \leq 2$ and $\eta \leq (2/q-1)$:

$$\langle 2\epsilon\rangle_{\text{axial}} = (P^2/S^2)a^2[(\tfrac{1}{1680}-\tfrac{1}{720}\eta^{-1}+\tfrac{1}{504}\eta^{-2}-\tfrac{1}{120}\eta^{-3}+\tfrac{1}{8}\eta^{-4}a^{-1}-\tfrac{7}{360}\eta^{-4}-\tfrac{7}{180}\eta^{-5})\cot 2\varphi-(-\tfrac{1}{384}\eta^{-1}+\tfrac{1}{160}\eta^{-2}$$
$$-\tfrac{1}{72}\eta^{-4})\csc 2\varphi]/[\tfrac{1}{120}-\tfrac{1}{24}\eta^{-1}+\eta^{-2}a^{-1}-\tfrac{1}{12}\eta^{-2}-\tfrac{1}{6}\eta^{-3}]. \tag{26}$$

The aberrations caused by spectral dispersion, refraction, and variation of response with wavelength have not been considered.

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